Examples of complex reactive flow applications

- Energy production by <u>nuclear</u> reactions

  Computational astrophysics, inertial confinement fusion,

  nuclear reactor design

- Energy production by <u>chemical</u> reactions

  Internal combustion engines, gas turbines, industrial

  burners and boilers, chemical propellants, incinerators,

  SCRAMJET and hypersonic jet engines

An Example Simulation Center for Engine Design

- Address problems with similar physics and chemistry features to ASCI and SBSS applications problems
- Issues related to parallel computing should be involved
- Problems are essentially 3-dimensional
- Multiphase flow systems
- Turbulence is a central technical problem
- A multidisciplinary team approach is required
- Problems involve all three DP national laboratories

Hydrodynamics

- Three dimensional, time - dependent
- Structured grids for some applications

  e.g., fuel / air mixing

- Unstructured grids

  e.g., full system with moving pistons and valves

- Gridless methods
- Scalable to massively parallel architectures

Relationship of reactive flow modeling to ASCI

"You are developing computational models for nuclear weapons simulations that you can never test. Can you develop comparable models for unclassified systems that can be tested and validated?"

Professor Steve Koonin, Provost, California Institute of Technology
National Security Advisory Committee
November 26, 1996
paraphrased

Chemical and nuclear reaction rates

General form for reaction rates:

$$k = C1 * C2 * \exp(-E / RT)$$

- Nuclear C1 and C2 refer to D, T, neutrons etc.
- Chemical C1 and C2 refer to hydrocarbons, OH, O, and other chemical radical species
- Both involve solution of implicit, stiff differential equations
- Both require transport and reactions of multi-species mixtures

Transport physics modeling

Chemical systems:

Transport via advection and diffusion for fuel, oxidizer, product and intermediate chemical species

Examples: C_3H_8, O_2, CO_2, OH, HO_2, NO

Typical number of species 50 - 100 (600)

Nuclear systems:

Transport via advection and diffusion for fuel, product and intermediate species

Examples: DT, He4, n, Pu239, fission products

Typical number of species 50 - 100

Transport physics required

- Species transport

  Reactions, product species, advection and diffusion

- Radiation transport

  Furnaces, soot, diesel engines, diagnostics

- Particle transport

  Spray injection

- Need for algorithm development, model integration
- Need for MPP techniques and formulations

Requirements for multiple physics models

Engines and furnaces:

- **Reactant mixing**
- **Reaction rates**
- **Multiphase flows**
- **Hydrodynamics**
- **Pollutant and trace species emissions**
- **Turbulent flows and reaction rates**
- **Moving boundaries, surfaces**
- **Ignition, critical phenomena**
- **Massively parallel computing**

Computer science needs

- Domain decomposition
- Load leveling
- Object - oriented programming
- Mesh and problem generation
- Computer languages   C, C++
- Program development environment
- Visualization of results
- Others

Logical steps for model development

- Start with hydrodynamics foundation
- Establish computational core
- Add physics and chemical submodels as needed for applications
- Establish and develop interactions with experimental programs
- Test submodels within overall code structure
- Refine submodels

Simulation Development Roadmap
Step 1

Air Intake and fuel injection

- **Aerosol or spray formation and vaporization**
- **Turbulent mixing of fuel and air**
- **Multiphase flow predicition**
- **Formation of viscous wall layers**
- **Equation of state**
- **Wall heat transfer**

Simulation Development Roadmap
Step 2

Compression of fuel - air mixture

- **Compressible turbulence with heat and mass transport**
- **Kinetic reaction modeling (preignition and knock)**
- **Wall heat transfer**
- **Surface chemistry simulation**
- **Liquid fuel vaporization and mixing**
- **Equation of state**
- **Closing of intake valves or ports**

Simulation Development Roadmap
Step 3

Ignition and Combustion

- **Plasma arc formation and expansion**
- **Chemical kinetics, stiff equations**
- **Radiation transport**
- **Coupled hydrodynamics and energy release**
- **Turbulent mixing of reactants and products**
- **Surface kinetics modeling**
- **Soot formation**
- **Equation of state**

Simulation Development Roadmap
Step 4

Expansion stroke

- **Wall heat transfer**
- **Coupled chemical kinetics and radiation**
- **Turbulent heat and mass tranport**
- **Roll-up vortex and crevice volume mixing**
- **Surface chemistry**
- **Soot production and destruction**
- **Chemical pollutant species production**

Simulation Development Roadmap
Step 5

Exhaust cycle

- **Kinetic reactions in exhaust port**
- **Surface chemistry**
- **Soot evolution**
- **Pollutant oxidation in catalyst**
- **Equation of state**
- **Heat transfer**
- **Materials physics**

Organizational Concept

- Program centered at a single university
- Multidisciplinary collaboration involving relevant departments

  e.g., Mechanical Engineering, Chemistry, Computer Science
  Applied Mathematics, Physics
- Involvement of other universities is encouraged
- Close collaboration with DP National Laboratories important
- Establish connections and access to MPP facilities
- Develop collaborations with industrial engine design programs